Resolving Statistical Uncertainty in Correlation Dimension Estimation

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Quantifying the connectivity of scale-free and biological networks

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Abstract

Scale-free and biological networks follow a power law distribution $p_k \propto k^{-\alpha}$ for the probability that a node is connected to k other nodes; the corresponding ranges for α (biological: $1 < \alpha < 2$; scale-free: $2 < \alpha \leqslant 3$) yield a diverging variance for the connectivity k and lack of predictability for the average connectivity. Predictability can be achieved with the Rényi, Tsallis and Landsberg–Vedral extended entropies and corresponding "disorders" for correctly chosen values of the entropy index q. Escort distributions $p_k \propto k^{-\alpha q}$ with $q > 3/\alpha$ also yield a nondiverging variance and predictability. It is argued that the Tsallis entropies may be the appropriate quantities for the study of scale-free and biological networks.

1. Introduction

The spread of infectious diseases, whether these be of a biological nature or computer viruses, depend on what are commonly referred to as network properties, how the nodes (populations, individuals) are connected to each other [1–3], as well as the statistical characteristics of the connections. Scale-free networks [2–5] are particularly notorious, since the connectivity, the number of other nodes to which each node is connected, has a finite mean but a diverging variance [3,6,7]. These properties imply not only the lack of an epidemic threshold for infinite networks (a threshold does exist for finite networks [2]), with all the corresponding dire consequences for the spread of disease, but also the inability to accurately quantify or predict the statistics of connectivity properties. This is unfortunate to say the least since the mean connectivity is one of the principle determinants of the spread of infection. On the other hand, the "disorder" [2] corresponding to the Shannon or information-theoretic entropy of the probability distribution appropriate to scale-free networks vanishes in the limit of infinite networks [8]. Since "disorder" may be interpreted as an inverse measure of predictability, this indicates that it might be possible to establish the mean connectivity with appropriate statistics, although the usual statistics of the information-theoretic entropy are obviously not sufficient since they yield a diverging variance for scale-free networks. Recent work [9] on the "disorders" corresponding to the extended

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[2] As usual, "disorder" written in quotes refers to the mathematically defined quantity; without the quotation marks, it is the general concept which is referred to.

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entropies of Rényi [10], Tsallis [11] and Landsberg–Vedral [12–15] (''normalized Tsallis entropies'' [16]) show that the connectivity properties of scale-free networks may be made predictable by a judicious choice of entropy and entropy index. This is confirmed by a finite mean and finite variance for the corresponding escort distributions [17]. We stress that the question we are addressing is the predictability of the average connectivity $\langle k\rangle$ of scale-free networks. We do not directly attack the spread of infection on these networks. Since $\langle k\rangle$, however, plays a major role in determining the spread, an accurate estimate for $\langle k\rangle$ is essential.

In general the spread of infection on different types of networks—''small world'' networks [1,18,19] (exponential [18], random [20] or scale-free [4,5]) or structured networks on lattices [21]—will show different behaviors. In this contribution we deal primarily with scale-free networks, for which the probability that a node (population or individual) is connected to k other nodes is given by $p_k \propto k^{-\alpha}$, $2 < \alpha \leqslant 3$ [2,3]. It is these constraints on α along with the power law distribution which ensure that the average connectivity $\langle k\rangle$ is finite, but yield a diverging variance. Maximum likelihood estimations of α indicate that α may be greater than 3 for sexually transmitted diseases [22,23], however. Then the variance remains finite. Furthermore, for other types of biological networks, involving genes, proteins and metabolism, α seems to lie between 1 and 2 [24]. In these cases, both the average connectivity $\langle k\rangle$ and the variance diverge. To cover all these cases, we consider the range $\alpha > 1$, not just $2 < \alpha \leqslant 3$, in our analyses.

To be explicit about the goal of the work presented here the basic statistical properties of continuous power law distributions for infinite networks are summarized in Table 1. The probability distribution is

$$p_k = \frac{(1-\alpha)k^{-\alpha}}{K^{(1-\alpha)}-1}, \quad 1 \leqslant k \leqslant K \tag{1}$$

The case $\alpha = 1$ is recovered by l'Hopital's rule. The mean connectivity $\langle k\rangle$ and the second moment $\langle k^2\rangle$ are calculated in the standard manner:

$$\langle k\rangle = \int_1^K k p_k \,\mathrm{d}k, \quad \langle k^2\rangle = \int_1^K k^2 p_k \,\mathrm{d}k \tag{2}$$

The variance $s^2 = \langle k^2\rangle - \langle k\rangle^2$, the standard deviation s and the coefficient of variation $c_v = s/\langle k\rangle$ follow. The major difficulty arises for scale-free networks ($2 < \alpha < 3$) with finite mean connectivity but diverging variance, standard deviation and coefficient of variation. These properties suggest an inability to accurately quantify or predict the mean connectivity. Regardless of how large a sample is used to obtain an estimate for $\langle k\rangle$ one has no idea how good an estimate it is. Any confidence level will simply yield $-\infty < \langle k\rangle < \infty$, rather obviously, for the confidence interval. Put another way, with a divergent variance an infinite number of (laboratory or numerical) experiments would be necessary to be sure that any finite proportion of the behaviors available to the system has been studied. Regardless of how many experiments are carried out, there are still an infinity of systems with the same $\langle k\rangle$ which have not been studied.

We will overcome this problem by turning to nontraditional statistics associated with the extended entropies of Rényi [10], Tsallis [11] and Landsberg–Vedral [12–16]), which are defined in various ways in terms of $Q \equiv \sum_k p_k^q$, where p_k is the probability of state k, and the parameter q may be referred to as the entropy index. We use the corresponding ''disorders'' [9] as inverse measures of predictability, since they circumvent any problems caused by any extensivity of the entropies. When a ''disorder'' vanishes, predictability is maximum, and we can surmount the difficulties in quantifying the mean connectivity caused by a diverging variance. This is seen clearly from the appropriate escort distribution [17], $\tilde{p}_k \propto p_k^q \propto k^{-q\alpha}$; if we choose $q\alpha \geqslant 3$, then both the mean and the variance of the escort distribution are finite.

Table 1
Basic statistical properties of continuous power law distributions in the infinite limit

	$\lim_{K\to\infty}\langle k\rangle$	$\lim_{K\to\infty} s$	$\lim_{K\to\infty} c_v$
$\alpha < 1$	$\frac{(1-\alpha)}{(2-\alpha)}K$	$\sqrt{\frac{(1-\alpha)}{(3-\alpha)(2-\alpha)^2}}K$	$\sqrt{\frac{1}{(1-\alpha)(3-\alpha)}}$
$1 < \alpha < 2$	$\frac{(\alpha-1)}{(2-\alpha)}K^{(2-\alpha)}$	$\sqrt{\frac{(\alpha-1)}{(3-\alpha)}}K^{(3-\alpha)/2}$	$\frac{(2-\alpha)^2}{(\alpha-1)(3-\alpha)}K^{(\alpha-1)/2}$
$2 < \alpha < 3$	$\frac{(\alpha-1)}{(\alpha-2)}$	$\sqrt{\frac{(\alpha-1)}{(3-\alpha)}}K^{(3-\alpha)/2}$	$\sqrt{\frac{(\alpha-2)^2}{(\alpha-1)(3-\alpha)}}K^{(3-\alpha)/2}$
$3 < \alpha$	$\frac{(\alpha-1)}{(\alpha-2)}$	$\sqrt{\frac{(\alpha-1)}{(\alpha-3)(\alpha-2)^2}}$	$\sqrt{\frac{1}{(\alpha-1)(\alpha-3)}}$

In the next section power law distributions, the various entropies and "disorders", and their relation to predictability are briefly summarized. With the help of our previous work on power law distributions [9], we then address the question of quantifying the mean connectivity for scale-free and biological networks. Following that the connection to escort distributions is treated. Finally it is argued on the basis of these results and others that the statistics corresponding to the Tsallis entropies may be the most profitable for the study of these systems.

2. Background

The power law probability distribution for the number of connections a node makes with other nodes is

$$p_k = k^{-\alpha} \Big/ \sum_{k=1}^{K} k^{-\alpha}; \quad k = 1, 2, \ldots, K \tag{3}$$

where K is the maximum number of connections possible. We assume that every node makes at least a single connection with another node; if it does not, it may be removed from the network. When the network is large enough that the limit $K \to \infty$ is appropriate, the distribution becomes

$$p_{k,\infty} = k^{-\alpha}/\zeta(\alpha); \quad k = 1, 2, \ldots, K \tag{4}$$

where $\zeta(\alpha) \equiv \sum_{k=1}^{\infty} k^{-\alpha}$ is the Riemann zeta function.

We consider Rényi [10], Tsallis [11] and Landsberg–Vedral entropies [12–16]). The Rényi entropies are perhaps best know as the basis of the definition of multifractals [25,26]; the Tsallis entropies are particularly suited for the study of nonextensive systems and arise naturally for power law probability distributions $p_k \propto k^{-\alpha}$ [27]; the Landsberg–Vedral entropies were introduced as another example of the set of possible extended entropies. All three classes of extended entropies are necessary to characterize power law distributions in the entirety of the parameter space defined by α and q [9], and they all reduce to the classical Shannon or information entropy, $H_S = -\sum_k p_k \ln p_k$, in the limit $q \to 1$. It has been noted that the Tsallis entropies are all measures of disorder (randomness), in the sense that they achieve a maximum when all probabilities are equal and vanish when only one state is realized; i.e., when one p_k is 1 and all others vanish [28]; this applies equally well to the Rényi and the Landsberg–Vedral entropies. In a similar sense these entropies are also inverse measures of predictability: when only one state is realized, predictability is absolute and the entropies vanish; when all states are equally probable, predictability is at a minimum and the entropies are maximum.

Actually the entropies have a deficit as measures for predictability; they increase with the size of the system in general. Since there is no *a priori* reason why predictability should decrease with the size of a system, a better inverse measure of predictability is provided by the quantities referred to as "disorders". These were introduced by Landsberg [29,30] to circumvent analogous problems with the entropies as measures of disorder and have been extended and generalized in various ways [31–38]. "Disorder" is defined generally as entropy normalized to maximum possible entropy; in the simplest case, appropriate to our work here, the maximum possible entropy is just that corresponding to the equiprobable distribution (all p_k equal). "Disorder" then varies between 0 and 1, and 1—"disorder" is a measure of predictability.

The quantity $Q \equiv \sum_k p_k^q$ in terms of which the entropies are defined is

$$Q = \sum_{k=1}^{K} k^{-\alpha q} \Big/ \left(\sum_{k=1}^{K} k^{-\alpha} \right)^q \overset{K\to\infty}{\to} Q = \zeta(\alpha q)/[\zeta(\alpha)]^q \tag{5}$$

and the entropies are

$$\begin{aligned} &\text{Rényi}: \quad H_{\mathrm{R}} \equiv (\ln Q)/(1-q); \\ &\text{Tsallis}: \quad H_{\mathrm{T}} \equiv (Q-1)/(1-q); \\ &\text{Landsberg–Vedral}: \quad H_{\mathrm{L}} \equiv (1-1/Q)/(1-q) \end{aligned} \tag{6}$$

The maximum entropies occur for the equiprobable distribution, $p_k \propto 1/K;\ k = 1, 2, \ldots, K$:

$$\begin{aligned} &\text{Rényi}: \quad H_{\mathrm{R,max}} = \ln K; \\ &\text{Tsallis}: \quad H_{\mathrm{T,max}} = (K^{(1-q)} - 1)/(1-q); \\ &\text{Landsberg–Vedral}: \quad H_{\mathrm{L,max}} = (1-1)/K^{(1-q)}/(1-q) \end{aligned} \tag{7}$$

The "disorders", entropy/maximum entropy, are then

$$\begin{aligned}&\text{Rényi}: \quad \Delta_R = (\ln Q)/[(1-q)\ln K];\\ &\text{Tsallis}: \quad \Delta_T = (Q-1)/(K^{(1-q)}-1);\\ &\text{Landsberg–Vedral}: \quad \Delta_L = (1-1/Q)/(1-1/K^{(1-q)})\end{aligned} \tag{8}$$

As a reminder: it is $1-\Delta$ that we take as measures for predictability. We emphasize that all "disorders" Δ lie between 0 and 1. Even when the entropies H diverge as $K \to \infty$, the $H_{\max}$ also diverge in such a way that the Δ remain finite and defined.

For the network problem at hand, the probability distribution (1) is of course discrete. Nonetheless, from this point on we will use the results for the corresponding continuous distribution (Eq. (1)) in the limit of an infinite network ($K \to \infty$) [9]. The entropy definitions (Eq. (4)) remain the same, but $\lim_{K\to\infty} \sum_{k=1}^{K} k^{-x} = \zeta(x)$ is replaced with $\lim_{K\to\infty} \int_1^K k^{-x}\,\mathrm{d}k$ at all the appropriate places in the equations above. The continuous results are qualitatively correct for discrete distributions. However, we note that there may be quantitative disparities. Although the continuous approximation to discrete networks is often used [2,3], these disparities have rarely been pointed out.

3. "Disorders" and predictability

The three measures of "disorder", Rényi, Tsallis and Landsberg–Vedral, behave qualitatively differently, depending on the values of α and q [9], as summarized in Table 2:

- the Rényi "disorder" vanishes for $\alpha > 1$ and $q \geqslant 1/\alpha$, and is maximal (i.e., 1) for $\alpha < 1$ and $q \leqslant 1/\alpha$; only for $\alpha < 1$ and $q > 1/\alpha$ or for $\alpha > 1$ and $q < 1/\alpha$ does Δ_R show a dependence on α and q;
- the Tsallis "disorder" vanishes for $\alpha > 1$ and $q \geqslant 1$, and is maximal for $\alpha < 1$ and $q \leqslant 1$; only for $\alpha < 1$ and $q < 1$ or $\alpha > 1$ and $q > 1$ does Δ_T show a dependence on α and q;
- the Landsberg–Vedral "disorder" vanishes for $\alpha > 1$ and $q > 1$ and for $\alpha < 1$ and $q > 1/\alpha$; it is is maximal for $\alpha > 1$ and $q < 1/\alpha$ and for $\alpha < 1$ and $q \leqslant 1$; only for $\alpha < 1$ and $1 < q < 1/\alpha$ or for $\alpha > 1$ and $1/\alpha < q < 1$ does Δ_L show a dependence α and q.

These qualitative aspects of the "disorders" are the same for discrete and continuous distributions. It is only in the regions of parameter space where a given disorder depends explicitly on α and q that this dependence differs quantitatively for continuous and discrete distributions.

These behaviors of the various entropies are summarized in the next three figures. Fig. 1 shows which of the entropies correspond to maximum predictability ($\Delta = 0$), Fig. 2 shows which of the entropies correspond to minimum predictability ($\Delta = 1$), and Fig. 3 shows which entropies depend explicitly on α and q.

For the cases of scale-free and biological networks, $\alpha > 1$. Thus, for maximum predictability, one would choose $q < 1/\alpha$ and the Tsallis "disorder", $1/\alpha < q < 1$ and the Tsallis or Rényi "disorder", or $q \geqslant 1$ and the Rényi or Landsberg–Vedral "disorder". One would avoid the Landsberg–Vedral quantities for $q < 1/\alpha$, since they yield minimum predictability. On the other hand, insights into the properties of the network might be obtained by investigating the dependence of one or other of the "disorders" on α and q. To this end one would choose to study the Rényi

Table 2
The extended "disorders" for a continuous distribution in the limit $K \to \infty$

		Δ_R	Δ_T	Δ_L
$\alpha < 1$	$q \leqslant 1$	1	$(1-\alpha)^q/(1-\alpha q)$	1
$\alpha < 1$	$1 < q \leqslant 1/\alpha$	1	1	$(1-\alpha q)/(1-\alpha)^q$
$\alpha < 1$	$q > 1/\alpha$	$(1-\alpha)q/(q-1)$	1	0
$\alpha = 1$	$q < 1$	1	0	1
$\alpha = 1$	$q = 1$	0.5	0.5	0.5
$\alpha = 1$	$q > 1$	0	1	0
$\alpha > 1$	$q \leqslant 1/\alpha$	$(1-\alpha q)/(1-q)$	0	1
$\alpha > 1$	$1/\alpha < q \leqslant 1$	0	0	$1-(\alpha q-1)/(\alpha-1)^q$
$\alpha > 1$	$q > 1$	0	$1-(\alpha-1)^q/(\alpha q-1)$	0

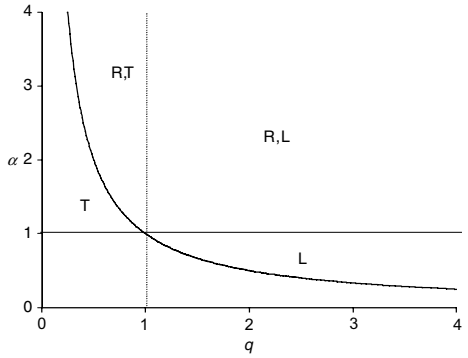

Fig. 1. Maximum predictability: parameter space for continuous distributions in the limit $K \to \infty$. Each region is labeled with the entropies which yield maximum predictability. R = Rényi, T = Tsallis, L = Landsberg–Vedral. The regions of parameter space are separated by the lines $\alpha = 1$, $q = 1$ and $\alpha q = 1$.

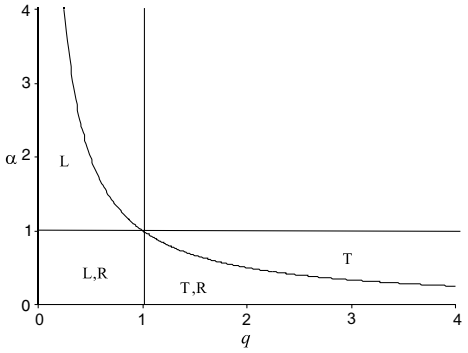

Fig. 2. Minimum predictability: parameter space. Otherwise as for Fig. 1.

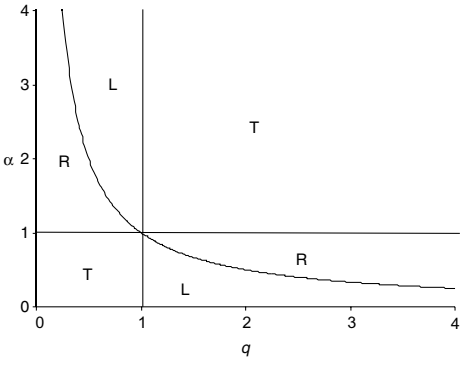

Fig. 3. Dependence: parameter space. Each region is labeled with the entropies which depend explicitly on α and q. Otherwise as for Fig. 1.

quantities for $q < 1/\alpha$, the Landsberg–Vedral quantities $1/\alpha < q < 1$ and the Tsallis quantities for $q > 1$. The dependence of the "disorders" on q for various values of α are shown in the Fig. 4.

- The Rényi "disorders" fall off from 1 to 0 as q increases from 0 to $1/\alpha$.
- The Landsberg–Vedral "disorders" fall off from 1 to 0 as q increases from $1/\alpha$ to 1.

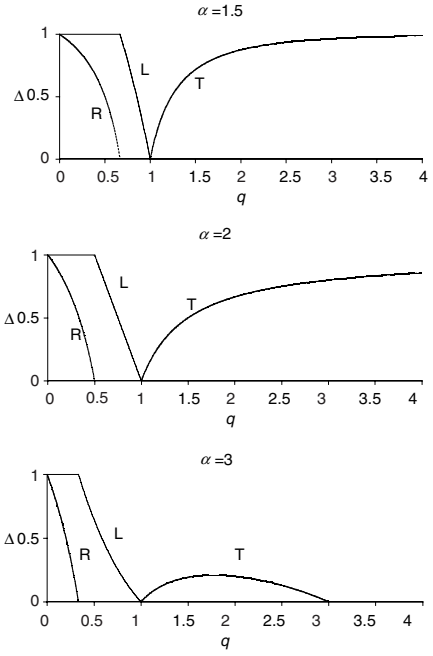

Fig. 4. The dependence of the various "disorders" on q for fixed α. R: Rényi; T: Tsallis; L: Landsberg–Vedral.

- For $\alpha \leqslant 2$, Δ_T increases monotonically with q for $q > 1$, but for $\alpha > 2$, Δ_T passes through a maximum at $q = 1/\alpha + 1/\ln(\alpha - 1)$ as q increases. This qualitative change in the dependence of Δ_T on q occurs at the value of α which just yields a finite $\langle k \rangle$ (i.e. at $\alpha = 2$).

4. Escort distributions and Tsallis statistics

Another way of achieving predictability for the connectivity properties of scale-free networks is through the trick of escort distributions [17]. One replaces the original probability distribution $\{p_i\}$ with the escort distribution $\{\hat{p}_i = p_i^q / \sum_i p_i^q\}$, here

$$\begin{aligned} &\text{discrete distributions}: \quad \hat{p}_k = k^{-\alpha q} \Big/ \sum_{k=1}^{K} k^{-\alpha q} \\ &\text{continuous distributions}: \quad \hat{p}_k = k^{-\alpha q} \Big/ \int_{k=1}^{K} k^{-\alpha q}\, \mathrm{d}k = (1-\alpha q) k^{-\alpha q} / [K^{(1-\alpha q)} - 1] \end{aligned} \tag{9}$$

Note that the denominator is just the quantity Q used to define the extended entropies and "disorders". For predictability we want a finite mean $\langle k \rangle$, which requires $\alpha q > 2$ and a finite variance, which requires $\alpha q > 3$. In other words, predictability can be achieved for both scale-free ($2 < \alpha q \leqslant 3$) and biological networks ($1 < \alpha q < 2$) by choosing $q > 3/\alpha$. In both cases this yields $q > 1$. For these values of q and α, it is the Tsallis "disorders" which show a dependence on q and α, and which are suitable for studying statistical properties. This argument is strengthened by Denisov's [27] demonstration that power law distributions follow from a maximum entropy principle for the Tsallis entropies with $q = 1 + 1/\alpha$. For $\alpha q > 3$, this implies $\alpha > 2$, i.e. scale-free networks.

By choosing $q > 3/\alpha$ one avoids the problem posed for the predictability of connectivity properties by a divergent variance, while at the same time a tool is available for studying generalized statistics. The possibility of replacing a divergent variance with a finite variance through an escort distribution is important for the reason mentioned in the introduction. With a divergent variance an infinite number of experiments would be necessary to be sure that any finite proportion of the behaviors available to the system have been studied. With a finite variance it is possible to determine the number of experiments necessary to cover any desired fraction of all possible cases. As a concrete example we choose $\alpha = 2.5$. For a nondiverging variance, we must have $q > 6/5$; the Denisov value is $q = 1 + 1/\alpha = 1.4$, which is

greater than the minimum q. By choosing a q yielding a nondiverging variance, predictability is achieved by using the Rényi or Landsberg–Vedral entropies, and the dependence of the statistics on q can be studied with the Tsallis "disorders".

When all these considerations are taken into account there is a case to be made that the Tsallis entropies and "disorders" offer the most profitable tools. (1) The Tsallis entropies were motivated by the study of nonextensive systems, for which the entropy does not scale with the size of the system; scale-free networks are just such systems. (2) Power law distributions follow from a minimum (Tsallis) entropy principle. (3) The value of q which yields minimum entropy leads to a finite $\langle k \rangle$ and variance, therefore achieving predictability for $\langle k \rangle$. (4) Finally, Abe [16] has argued that only the Tsallis entropies are stable (in a restricted sense—our comment) for power law distributions.

5. Concluding remark

The critical reader may have asked if we have not set up a straw man here. After all, it is α which is usually determined from data analyses and $\langle k \rangle$ is then calculated from α (Table 1). Then the problem of a diverging variance for k does not arise, insofar as estimates of $\langle k \rangle$ go. However, since $\langle k \rangle$ can be calculated from α, α can be calculated from $\langle k \rangle$, and an inability to estimate $\langle k \rangle$ because of a diverging variance should make one suspicious of the reliability of estimates of α. That this suspicion is justified is illustrated by studies of the number of sexual partners, relevant to sexually transmitted diseases. Different groups [2,3] have found power law distributions with $2 < \alpha < 3$, i.e. scale-free networks, presumably from linear regression of the logarithmic form of the distribution $p_k \propto k^{-\alpha}$. Jones and Handcock [22,23] have criticized this estimation procedure, however. They turned to maximum likelihood estimates and found $\alpha > 3$, which is no longer in the range consistent with scale-free networks. If there is uncertainty in the estimate of α, then uncertainty remains in the estimate of $\langle k \rangle$ even when it is calculated from α, and the problems caused by a diverging variance for k have not been avoided. These can be avoided, however, by the procedures we advocate here: analysis of the escort distribution and Tsallis or Rényi "disorders" for a sufficiently large q.

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